

## 不等长批次过程的有序时段划分、建模及故障检测

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**摘要:** 对具有不等长时段的多时段批次过程进行监测是十分重要而且具有一定难度的. 时段在批次间的错位现象导致时间方向的不同过程特性混合在一起, 这给时段分析以及在线应用带来了一系列的问题. 为了解决不等长所带来的问题, 本文提出一种基于不等长时段有序识别及建模的故障检测方法. 该方法的主要贡献包括以下方面: 1) 该方法通过步进地衡量过程的变量相关性对模型精度以及监测性能的影响, 自动有序地识别出每个不等长时段; 2) 在每个时段内, 通过对不规则的过程数据进行整合建立了时段模型以捕捉不规则的时段特性; 3) 本文提供了一种简单而有效的在线判断新样本隶属时段和监测其运行状态的方法. 最后, 本文通过一个实例—具有不等长批次长度的注塑过程阐述了本方法的有效性.

**关键词:** 批次过程; 不等长批次; 不等长时段识别; 多元统计建模; 故障检测

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## Sequential unequal-length phase identification and modelling method for fault detection of varying-duration batch processes

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**Abstract:** The work of monitoring multiphase batch processes with unequal phase durations is of great importance but difficult. Due to misaligned phases, process characteristics are mixed along time direction which causes problems in phase analysis and modeling as well as online application. In order to solve the uneven-length problem, this paper proposes a sequential unequal-length phase identification and modeling-based fault detection method. The main contribution of the proposed method includes: 1) multiple unequal-length phases are sequentially identified by evaluating the changes of process variable correlations step-wise regarding their influences on model accuracy and monitoring performance; 2) irregular phase characteristics are captured by irregular data-arranging-based modeling strategy; 3) the proposed method provides an easy but effective way to judge the phase affiliation and check the operation statuses of new samples in real time. Its online monitoring performance is illustrated by an injection molding process with varying durations.

**Key words:** batch processes; varying batch durations; unequal-length phase identification; multivariate statistical modeling; fault detection

### 1 Introduction

Batch processes play a significant role in modern industrial manufacturing, the work of monitoring these batch processes is very important to ensure safe production and consistent high-quality products. However, since first-principles based model is hard to build, data based multivariate statistical analysis methods<sup>[1-5]</sup> have attracted rising attentions. Among them, multi-way principle analysis (MPCA) and multi-way partial least regression (MPLS), which were proposed by Nomikos and Macgregor<sup>[4-5]</sup>, extend the applications of traditional multivariate statistical analysis methods

from continuous processes to batch processes. Since then, more and more researches<sup>[6-8]</sup> have been conducted around statistical modelling and monitoring for batch processes.

However, most researches are based on the idealized assumption that batches have equal durations, which cannot be well satisfied in real industrial manufacturing processes due to the different operation conditions and alternative product targets. In particular, for multiphase batch processes, the lengths of phases may be different over batches and the resulting irregular phase data cannot directly be used for statistical analysis

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and modelling. Therefore, many studies have been conducted to handle uneven-length batch processes<sup>[9–17]</sup>. The above methods can be divided into two types: direct signal synchronization methods<sup>[9–15]</sup> and irregular phase partition based modelling methods<sup>[16–17]</sup>.

Direct signal synchronization means batch trajectories are synchronized by performing some signal processing strategies. The simplest methods<sup>[9]</sup> include cutting the trajectories of all batches to the shortest one and expanding the trajectories, which are only suitable when the main process characteristics are captured in their common parts. A reasonable alternative method<sup>[10]</sup> is to synchronize process trajectories according to an indicator variable. However, it may distort the original process variable correlations. Besides, for multiphase batch processes, the changes of phase characteristics may not be correctly indicated by an indicator variable. Other methods<sup>[13–15]</sup> for handling the uneven length problem include Dynamic Time warping, Correlation Optimization Warping and so on. In general, these methods treat the whole batch as a single subject and ignore the multiphase nature. For multiphase batch process, even after the batch lengths are synchronized, the phases are in fact misaligned over batches. Thus process characteristics cannot be well reflected since data belonging to different phases are mixed and analyzed together.

To overcome the limitations of direct signal synchronization methods, Lu et al.<sup>[16]</sup> proposed the sub-phase division methods for handling uneven-length problem of multiphase batch processes. Two models were built, in which, one was for phase division and another for monitoring model developments. While Lu's method has been demonstrated effective and applied successfully, it may have some drawbacks during the phase partition procedure. First, the clustering algorithm was used for irregular phase partition and it did not consider the time sequence of process operation, which may result in improper phase model as well as may lead to a disordered phase partition results. Besides, the clustering based phase partition method takes the whole time-slice as the basic analysis unit, which thus may not correctly reveal the phase shift of some specific batches in this time-slice. Zhao et al.<sup>[17]</sup> developed phase division and modeling method for batch processes with serious uneven-length problem in which, different unequal groups were separated since they have quite different characteristics. However, for each unequal group, phases are still identified using clustering algorithm and drawbacks of clustering based method as mentioned above may also exist.

To address the unequal-length problem, this article proposes a sequential unequal-length phase identification and modelling method for fault detection of

uneven-length multiphase batch processes. The major contribution is specified as follows: 1) Irregular phases are automatically identified by detecting the changes of variable correlations as evaluated by one statistical monitoring index. 2) Based on the phase partition results, phase models can be developed by data rearrangement strategy and then local process characteristics are well described. 3) During online application, the phase affiliation of samples will be real-time judged so that the proper phase model can be adopted to distinguish between real fault and phase shift.

What's more, it is noted that SSPP algorithm is only suitable for the equal-length batches while the proposed method is able to solve a more general problem, that is, unequal-length batch problem. In other words, SSPP algorithm can be regarded as one special case of the proposed method.

## 2 Methodology

### 2.1 Data preparation

In general, before modelling, data should firstly be normalized. There are two common approaches for data normalization in batch process industry: variable-unfolding based method and batch-unfolding based method<sup>[18]</sup>. Due to the misaligned data caused by uneven phases, normal batch-wise variations cannot be well reflected by batch-unfolding based method. While variable-unfolding based method can handle uneven batch data, more variations will be covered simultaneously, and thus the resulting confidence region can be very wide, which makes the model insensitive to small variations. Accordingly, the advantages of the two methods can be combined and utilized in the proposed algorithm. Variable-unfolding based method is only chosen for phase partition, and batch-unfolding based approach will be adopted later for monitoring system development.

In each batch run (batch index  $i = 1, 2, \dots, I$ ), assume that  $J$  process variables are measured online at  $k = 1, 2, \dots, K$  time intervals throughout the operation cycle where the duration is not fixed in length, forming each batch set, denoted as  $\mathbf{X}_i(K_i \times J)$ . Then, batch set  $\mathbf{X}_i(K_i \times J)$  are aligned from top to bottom and keep the dimension of variable unchanged, giving an  $\sum_i^I K_i \times J$  matrix  $\mathbf{X}(\sum_i^I K_i \times J)$ . Subsequently,  $\mathbf{X}(\sum_i^I K_i \times J)$  is normalized by subtracting the means and dividing by the standard deviations. Then normalized time-slices  $\mathbf{X}_k(I_k \times J)$  can be separated from  $\mathbf{X}(\sum_i^I K_i \times J)$ . At the end of the batch process, time-slices contain different numbers of batches due to the uneven problem.

## 2.2 Phase division by sequentially analyzing variable correlations

The basic idea of the proposed method is to evaluate samples of each batch sequentially along time direction starting from the initial phase model and check the changes of variable correlations. The initial phase model is developed based on the first time-slice where batches have similar characteristics and then will be updated by including more and more samples with similar process characteristics. If samples with different characteristics are included, then the accuracy of the representative model will be decreased, which indicates the ending of the current phase for the related batches. Correspondingly, by sequentially evaluating the changes of variable correlations from the beginning of the process, phase landmarks of each batch can be automatically identified. The specific procedure is presented as follows.

**Step 1** Input the normalized time-slice data  $\mathbf{X}_k(I_k \times J)$ .

**Step 2** Initial phase model development. Develop an initial monitoring model  $\mathbf{P}_{v,1}(J \times R)$  by performing PCA algorithm on the first time-slice data matrix, here termed as  $\mathbf{X}_{v,1}(I_1 \times J)$ .

$$\mathbf{X}_{v,1} = \mathbf{T}\mathbf{P}_{v,1}^T + \mathbf{E} = \sum_r^R \mathbf{t}_r \mathbf{p}_r^T + \mathbf{E}, \quad (1)$$

$$\mathbf{T} = \mathbf{X}_{v,1} \mathbf{P}_{v,1},$$

where  $v$  means that time-slice data is variable-unfolded, if there is only one time-slice,  $\mathbf{X}_{v,k}(\sum_1^k I_k \times J)$  equals to  $\mathbf{X}_k(I_k \times J)$ .  $\mathbf{P}_{v,1}$  will work as the initial phase model to evaluate the variable corrections of the following samples of each batch. Then calculate the monitoring statistic values of squared prediction errors (SPE) and determine the confidence limit  $\text{Ctrl}_{v,1}$ . A looser confidence limit should be set up for two reasons: First, time-wise variations are larger and more complex; Second, monitoring model based on first time-slice or several time-slices cannot cover the whole phase information. Thus  $\alpha$  is selected to enlarge the confidence limit, which determines how much difference of variable correlations is allowed for the neighboring samples within the same phase. How to choose the value of  $\alpha$  depends on the specific process characteristics. In general, larger  $\alpha$  value means more difference of variable correlations is allowed and the accuracy of phase model will be decreased since different variations should be simultaneously captured by one representative model; smaller  $\alpha$  value means that more irregular phases will be obtained and more accurate monitoring models will be developed to describe each sample.

**Step 3** Variable correlation evaluation. The current model  $\mathbf{P}_{v,1}(J \times R)$  is adopted to monitor each batch of the next time-slice and SPE statistic is calculated for evaluating variable correlations.

$$\begin{cases} \mathbf{t}_i = \mathbf{P}_{v,1} \mathbf{x}_i, \\ \mathbf{e}_i = \mathbf{x}_i - \mathbf{P}_{v,1}^T \mathbf{t}_i, \\ \text{SPE}_i = \mathbf{e}_i^T \mathbf{e}_i, \end{cases} \quad (2)$$

where subscript  $i$  represents the  $i$ th batch of the next time-slice. If there are batches showing consecutive three alarming signals by adopting the current monitoring model, then these batches are “abnormal”, which means their variable correlations are changing significantly and may enter the next phase. Then record the first alarming time  $k_i$  of these batches and batch data before  $k_i$  are denoted as one sub-phase. Otherwise, it means the whole time-slice is operating in the “normal” condition. Here, “normal” means the process is in the current phase.

**Step 4** Phase model updating. Add the “normal” batches of the next time-slice into the modeling data of current monitoring model and variable-unfold them,  $\mathbf{X}_{v,2}(\sum_1^2 I_k \times J)$ . Perform PCA on the variable-unfolded data  $\mathbf{X}_{v,2}(\sum_1^2 I_k \times J)$  to update monitoring model  $\mathbf{P}_{v,2}(J \times R)$  and confidence limit  $\text{Ctrl}_{v,2}$ . The updated model is then utilized to monitor batches of the next time-slice.

**Step 5** Phase landmark determination. Repeat Steps 3 and 4 until the first phase has been identified for every batch.

**Step 6** Recursive implementation. Remove the first sub-phase, the remaining data are aligned and employed as the new input in Step 2. Then repeat Steps 2–5 to determine the following phases.

By sequentially checking the changes of variable correlations for each batch, irregular phases are identified in order. It is noted that the general uneven problem is focused on in this work, where the process characteristics over irregular batches within the same phase can still be modelled by a representative phase model.

Furthermore, the specific of difference between the proposed partition method and that in Ref. [8] is described as below. SSPP algorithm in Ref. [8] takes the whole time slice as the basic analysis unit since batch length is equal. In this way, the phase landmarks of all batches are identified at the same time. In contrast, the proposed method analyses each sample within time slice separately since phases are misaligned over batches, which is more reasonable for the uneven-length case considered here.

## 2.3 Data re-arrangement for sub-phase model development

Since uneven-length batch process has been divided into several phases and the uneven batch information of each phase such as the shortest length  $k_s$  as well as the longest length  $k_l$  have also been determined, phase-

based monitoring model can then be developed. Before developing sub-phase models, data normalization should firstly be carried out. Batch-unfolding based method are adopted because process characteristics stay similar among time-slices within the same phase. What's more, for the irregular time-slice data (from  $k_s+1$  to  $k_1$ ) at the end of each phase, because insufficient batches are contained in each of them and reliable process information cannot be derived, they are unfolded variable-wise to construct a generalized time-slice. For samples during time region  $[k_s, k_1]$ , they are all represented by the generalized time-slice  $\mathbf{X}_k^w (\sum_{k_s}^{k_1} I_k \times J)$ .

Correspondingly, normalized data are prepared for the following sub-phase modeling.

After data normalization, the sub-phase data  $\mathbf{X}_c (\sum_1^{K_c} I_k \times J)$  are arranged by variable-wise unfolding the time-slices  $\mathbf{X}_k (I_k \times J) (k = 1, 2, \dots, K_c)$  within the same phase  $c$ . An unified phase model is subsequently developed.

$$\mathbf{X}_c = \mathbf{T}_c \mathbf{P}_c^T + \mathbf{E}_c = \sum_r^R \mathbf{t}_{c,r} \mathbf{p}_{c,r}^T + \mathbf{E}_c, \quad (3)$$

$$\mathbf{T}_c = \mathbf{X}_c \mathbf{P}_c,$$

where  $\mathbf{P}_c (J \times R_c)$  reveal the major variation directions captured within the current phase and  $R_c$  is the number of the retained PCs.  $\mathbf{T}_c$  are phase-representative scores.

Based on the unified phase model, related statistics can be calculated:

$$T_k^2 = (\mathbf{t}_k - \bar{\mathbf{t}}_k)^T \sum_c^{-1} (\mathbf{t}_k - \bar{\mathbf{t}}_k), \quad (4)$$

$$SPE_k = \mathbf{e}_k^T \mathbf{e}_k,$$

where  $\mathbf{t}_k (R_c \times 1)$  is the PC vector separated from  $\mathbf{T}_c (\sum_1^{K_c} I_k \times R_c)$  and  $\bar{\mathbf{t}}_k$  is the mean vector of  $\mathbf{T}_k (I_k \times R_c)$ , which are time-slice scores separated from  $\mathbf{T}_c (\sum_1^{K_c} I_k \times R_c)$ .  $\Sigma_c$  is the covariance matrix of  $\mathbf{T}_c (\sum_1^{K_c} I_k \times R_c)$ .  $\mathbf{e}_k (J \times 1)$  is the residual vector which is obtained from  $\mathbf{E}_c (\sum_1^{K_c} I_k \times J)$ .  $T^2$  statistic describes variations in the systematic part captured by monitoring models and SPE statistic reveals variable correlations.

For each phase, confidence limits can be defined at each time for the two monitoring statistics. Assuming the process data follows a multivariate normal distribution, so confidence limits can be determined by F-distribution and a weighed chi-squared distribution for  $T^2$  and SPE respectively<sup>[19]</sup>. However, considering the confidence limit of  $T^2$  established by F-distribution is not very sensitive, another way can be utilized to define confidence limit: arrange the values of monitoring statistic in a descending order at each time and choose

the value at 95% (or 99%) of the ordered data as the confidence limit.

## 2.4 Online phase judging and fault detection

For multiphase batch processes with unequal-length phases, process time index fails to judge the phase affiliation of new samples. Besides, the operation statuses of new samples will be more complex which can be divided into three cases: normal operation, abnormal operation and phase shift. So how to judge the phase affiliation of new samples and check their operation statuses in particular distinguish phase shift and real fault is of great significant during online monitoring. The specific procedure is as follows:

a) For the data within the region  $[1, k_s]$ , the phase affiliation of is certain and process time is sufficient to judge their phase affiliations. Then according to the process time index, proper phase model will be adopted and two statistics are calculated to check their operation statuses. If both statistics stay well in the confidence region, it means the new sample operates normally; otherwise, there may be process fault.

b) For the data during the region  $[k_s + 1, k_1]$ , sample may still lie in the current phase or shift to the next phase. Then the current phase model and the next phase model will be adopted in turn to monitor this sample. The specific phase which can well accommodate the current sample with no alarms will be chosen as the affiliation. If both phase models issue monitoring alarms, it is regarded as a process fault. Therefore, the phase shifts will be readily distinguished from abnormal behaviors.

## 3 Illustration and discussion

In this section, a typical multiphase batch process, injection molding, is used to illustrate the performance of the proposed algorithm. A typical injection molding process can be divided into three major operation phases: Firstly, injection of the plastic melt into the mold, followed by is packing holding of the plastic in the mold under pressure, and finally, cooling of the plastic in the mold. It can be easily set as a typical uneven-length multiphase batch process for experiments to verify the proposed phase identification and modelling method for online monitoring, where the injection phase duration is not fixed but rather depends on the injection velocity. Here, the injection velocity is artificially set to change from 22 to 26 mm/s, involving three typical velocity values: 22, 24, 26 mm/s. Correspondingly, the duration of injection phase ranges from 99–84 samples. It is clear that moderate uneven-length problem has been simulated. Here for simplicity, except the injection phase, other phases are controlled to have exactly the same duration. The material used in this work is high-density polyethylene (HDPE). Nine process variables are selected for modelling, totally 35 normal batches are collected under normal operation

conditions, where 23 batches are used for modelling. Besides, two types of faults are considered: Injection phase fault and packing-holding pressure fault.

As shown in Fig.1, the uneven injection phases have been automatically determined by the proposed algorithm without post processing. For comparison, real physical phases indicated by an indicating variable (here is screw stroke) have also been plotted. Fig.1(a) shows the phase partition results for modelling data while Fig.1(b) reveals the results of testing batches. It is obvious that using the proposed algorithm, the uneven injection phase results are basically in line with the real physical phases. What's more, a measurement index  $\Delta t = |\text{phase}_{\text{real}} - \text{phase}_{\text{partition}}|$ , has been defined to evaluate the accuracy of phase division results. The mean and mean absolute deviation (MAD) values of  $\Delta t$  are calculated for 23 modelling batches and 12 testing normal batches respectively. Table 1 shows the comparison of phase division accuracy between the proposed method and clustering-based method used in Ref. [17]. It is noted that the proposed method has better phase partition performance in comparison with the clustering-based method.

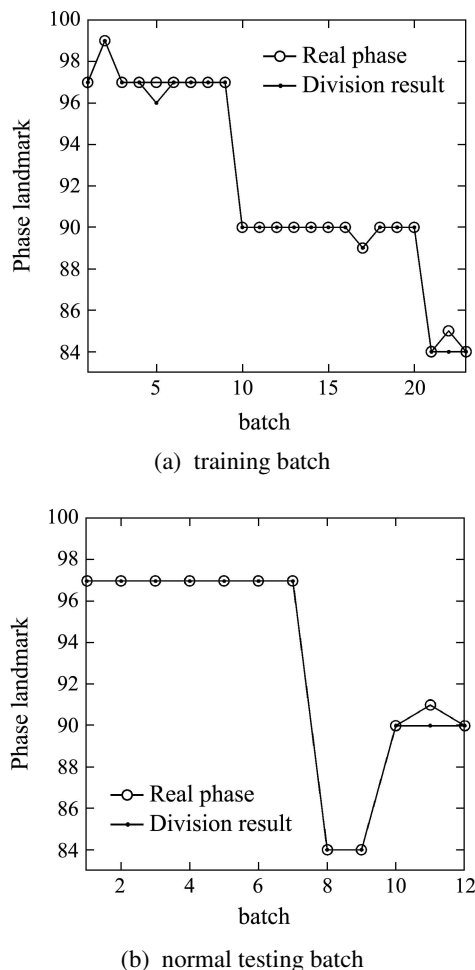


Fig. 1 Phase partition results of uneven injection phase by the proposed method

Table 1 Evaluation results of phase division accuracy ( $\Delta t$ ) between the proposed method and clustering based method

|          | Proposed method | Clustering-based method |
|----------|-----------------|-------------------------|
| Training | $0.13 \pm 0.23$ | $1.04 \pm 1.11$         |
| Testing  | $0.08 \pm 0.15$ | $1.17 \pm 1.08$         |

Based on the phase division results, different monitoring models are developed for each irregular phase. Monitoring results of injection phase and packing-holding phase are only presented here to illustrate the online monitoring performance of the proposed method. For samples before 85, injection phase model should be adopted and two monitoring index  $T^2$  and SPE will be calculated to check their operation status. If both of them are below the confidence limits, then process can be regarded as normal; for data during [85, 99], injection phase model is firstly adopted to check whether there is any alarming signal for  $T^2$  or SPE, if alarms occurs, packing-holding phase model is then utilized for monitoring; on condition that alarming signals still exist, then fault happens; otherwise, process just switches from injection phase to packing-holding phase. With regarding to data after 99, they are certainly beyond the injection phase and corresponding monitoring model can be adopted according to time index for online monitoring.

Table 2 shows the monitoring performance results of injection phase and packing-holding phase respectively. FAR (false alarming rate) of  $T^2$  and SPE are calculated for normal testing batches. One FAR is calculated for 12 batches where the total number of false alarming signals is divided by the total number of samples from 12 batches. Obviously, FAR of SPE fluctuate around 5% and are less than 8%, which agree with the 95% confidence limit. While for  $T^2$ , FAR are much smaller for the reason that phases are identified according to variable correlations evaluated by SPE, so  $T^2$  is not so sensitive as SPE for online monitoring. What's more, it is noted that FAR do not show significantly differences between injection phase and packing-holding phase, indicating phase partition results are reliable to certain extent.

Table 2 Online monitoring performance (FAR%) for normal case for two phases

|       | Injection phase | Packing holding phase |
|-------|-----------------|-----------------------|
| SPE   | $2.13 \pm 2.84$ | $4.14 \pm 2.86$       |
| $T^2$ | $1.29 \pm 1.93$ | $1.07 \pm 1.07$       |

Figure 2 demonstrates SPE monitoring chart for phase switch. Real phase switch occurs at the 91st sample interval, from injection phase to packing-holding phase. It is clear that SPE index continuously exceeds the confidence limit at 91st sample by adopting injec-

tion model, and then alarming signals have been eliminated by using packing-holding phase model. For  $T^2$ , there is similar result which is not shown here. Be-

sides, for fault test batches, reliable fault detection performance can also be obtained. The monitoring charts are not presented as the length limit.

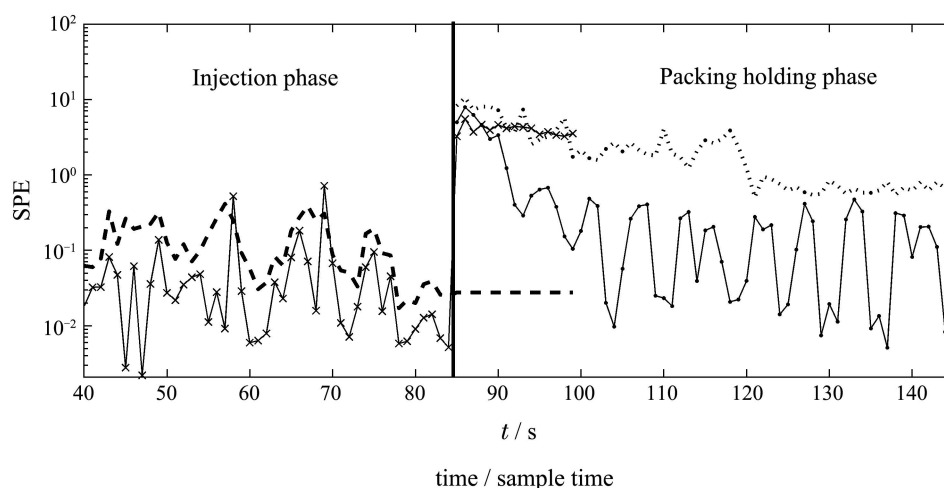


Fig. 2 SPE monitoring results for normal process switch using the proposed method (bold/ fine dash line: control limit of Injection/Packing holding phase; crossed/dot line: SPE statistic for Injection/Packing holding phase)

Table 3 shows the comparison results of on-line monitoring performance between the proposed method and Lu's clustering based method. In general, the proposed algorithm shows preferable monitoring performance than clustering-based method, which is evaluated by paired t-test ( $\alpha = 0.05$ ). For FAR, the average results of injection phase and packing holding phase are presented here. It is noted that with the 95% confidence level, FAR of the proposed method are almost around 5% with respect to SPE statistic compared with 3% of  $T^2$ , which also denotes that SPE is more sensitive and is the critical monitoring statistic in the proposed algorithm. While for fault batches,  $\Delta T = \text{FAT} - \text{FOT}$  (FAT: first alarming time; FOT: first occurring time) is calculated for evaluating fault detection performance. It is noted that both methods have small values of  $\Delta T$ , revealing good fault detection ability.

Table 3 Online monitoring performance comparison between the proposed method and clustering based method

|            |       | Proposed method | Clustering-based method |
|------------|-------|-----------------|-------------------------|
| FAR/%      | SPE   | $2.70 \pm 2.81$ | $7.86 \pm 4.68$         |
|            | $T^2$ | $1.18 \pm 1.01$ | $5.68 \pm 3.12$         |
| $\Delta T$ | SPE   | $4.00 \pm 1.96$ | $5.28 \pm 3.18$         |
|            | $T^2$ | $0.57 \pm 1.02$ | $3.80 \pm 3.76$         |

## 4 Conclusions

In the present work, a sequential unequal-length phase identification and modelling based fault detection method is proposed for multiphase batch pro-

cesses with varying durations. By evaluating the changes of variable correlations for each batch orderly along time direction, different underlying process characteristics are distinguished and irregular phases can be automatically identified without post processing. For sub-phase developments, irregular phase data are re-arranged and generalized time-slices are constructed. For online monitoring, phase affiliation can be real-time judged and phase shift can be well distinguished from process fault. The application to the injection molding process shows the effectiveness of the propose method.

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## 书 讯

科学出版社于2015年7月出版由黄琳院士等撰写的专著《中国学科发展战略·控制科学》一书, 该书是根据中国科学院信息技术科学部常委会确定的项目“控制科学学科发展战略”的一批学术报告经过充分研讨整理而成. 该书汇集了海内外近百名华人知名教授专家的智慧, 历时两年多最后定稿. 全书共分六部分: 第一部分是控制科学发展战略总体报告, 论述了控制科学的定位、新的时代特征带来的新特点和新方向; 分析了控制科学发展的历史和从中得到的启示; 从控制科学整体的角度对五个重要领域提出了新时代下具有挑战性的新问题; 对现今人类社会和我国控制科学的进一步发展进行了需求分析、学科发展的思考, 提出了进一步发展的几个重大需求方向和一些实质性的建议. 本书后五部分是控制科学关注的五个重要领域: 控制理论、航空航天与运动体控制、过程控制、网络控制、交叉学科、教育和其他的分组报告, 报告详细分析了这些领域的发展、需求、面临的挑战和新的机遇与问题.

本书具有以下重要特点: 从控制科学学科战略发展的角度出发, 充分分析了当今信息丰富时代的特征; 归纳总结了重大需求和学科的逻辑发展带来的关键科学问题; 分析了新的科技进展对控制科学发展提供的机遇和条件, 以及控制学科发展的瓶颈和新的可能的学科生长点等.

该书可供系统与控制科学、自动化相关领域、力学、应用数学、工程科学及与之相关的信息科学与工程应用领域的教学与科研人员、研究生和工程师阅读, 也可为科技与工程管理部门研究和制定学科发展规划提供参考.

(李倩)